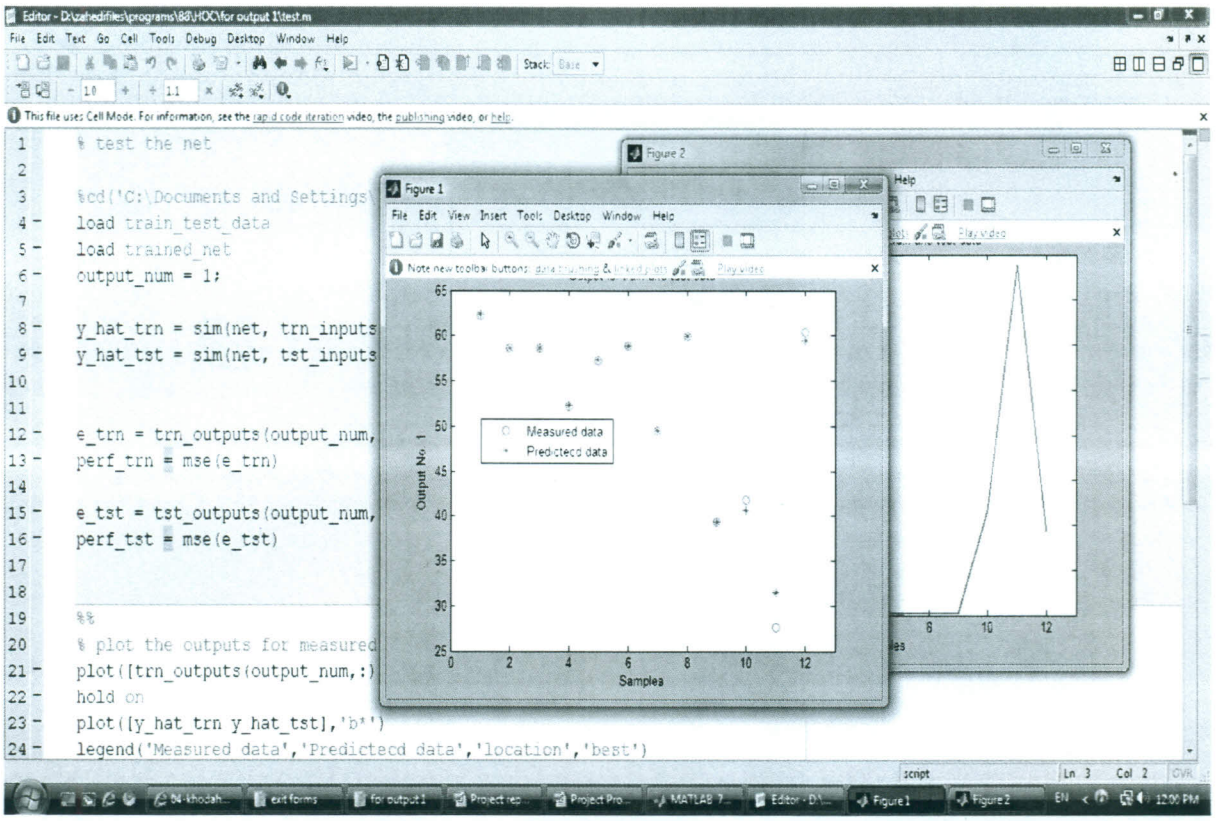

Simulation and optimization of heavy oil cracking (HOC) unit using neural network and genetic algorithm

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Abstract

This research presents an artificial neural network (ANN) model to investigate optimum operating condition of heavy oil catalytic cracking (HOC) to reach maximum gasoline yield. In this case, American petroleum institute index (API) , weight percentage of sulfur, Conradson carbon residue content (CCR), gas, coke, and liquid volume percent conversion (%LV) of reaction were considered as ANN model inputs while the percentage of normal butane (N-C_4), iso-butane (I-C_4), butene (C_4=), propane (C_3), propene (C_3=), heavy cycle oil (HCO), and light cycle oil (LCO) and gasoline (GASO) were considered as network outputs. 70% of all industrial collected data set were utilized to train and find the best neural network. Among the different networks, feed-forward multi-layer perceptron network with Levenberg Marquardt (LM) training algorithm with 10 neurons in hidden layer was found as the best network. The trained network showed good capability in anticipating the results of the unseen data (30% of the all data) of catalytic cracking unit with high accuracy. In the next step of study sensitivity analysis was carried out to find the effect of the operating condition on gasoline and products yields. Finally genetic algorithm (GA) was used to optimize neural model of the plant. It was found that gasoline yield can be increased to 73.6429 % by adjusting operating conditions.

1. Introduction

Conversion of heavy oil to light oil products has been important due to the low demand of heavy fuels and increasing demand of light fuels [1]. Heavy oil catalytic cracking (HOC) is one of fluid the catalyst cracking (FCC) processes. In early 1942, the process was operated in United States and so far many progresses have been obtained on developing and modifying of related catalysts and processes [2].

Comparing to thermal cracking, catalytic cracking generates more gasoline with higher quality (more octane number) and less coke. Unlike thermal cracking which can be operated with all type of feed, catalytic cracking uses only low metal content feeds., High temperature (500-530℃), low pressure (2-3 bar) and specific catalysts. Vacuum gasoil (VGO), visbreaked gasoil and the vacuum column residue with low metal content are the feed of catalytic cracking unit. Main products of FCC consist of gasoline (40-50%), LPG, a light cut of gasoil which is called light cycle oil (LCO), a heavy cut of gasoil called heavy cycle oil (HCO) and also some coke which is consumed in process [1,2].

Heavy feeds like atmospheric distillation residue are hardly refined. They are full of coke producing molecules. Excessive production of coke leads to significantly increase in regenerator temperature which causes damage to catalyst or regenerator tools. The amount of CCR content of heavy feeds is 2-8%. They are enriched of nickel and vanadium which cause undesirable effects on process catalyst and decrease catalyst selectivity. They are also enriched of hetro-atomic nitrogenated compounds which neutralize acidic sites of catalyst, and decrease its activity and play significant role in coke formation. HOC process is one of catalyst cracking processes which has been designed for treating this type of feeds [2].

2. Methodology

In order to construct a model of ANN, HOC unit data were collected from typical plant. To insure that the data cover the normal limits of operation data, the off data were removed from data list. Model variations and data limits are tabulated in Table 1.

Table 1.

In order to train and find the best ANN, all data sets were divided into two sections: train and test (generalization). 70% of all data were selected for train and the remaining 30% (unseen data) were selected for test. In this study for each output a separate network has been trained [27].

API, weight percentage of sulfur, CCR content, gas, coke and liquid volume percent conversion (%LV) of reaction are network inputs while network outputs include percentage of normal Butane (N-C_4), iso Butane (I-C_4), Butene (C_4=), Propane (C_3), Propene (C_3=), HCO, and LCO and gasoline (GASO).

3. Literature review

Several studies have been focused on FCC and HOC process [3-9]. Artificial neural network (ANN) with high training capability has many applications. During the recent 15 years, ANNs have been increasingly used because of their capability and ability to solve complicated problems. Process modeling and simulation especially while no analytical model exists, parameter estimation and optimization are among the applications of ANNs in chemical engineering [10, 11].

According to our literature survey, there are few studies on simulation and modeling of HOC units .In a novel computer simulation by Bolkan-Kenny et al. [12] it was found that FCC process downer reactors are slightly more beneficial than riser reactors when commercial silica-alumina catalysts are used.

Maciel Filho and Sugaya presented a computer aided tool for heavy oil thermal cracking process[13].They proposed a dual plug flow reactor representation for the light pyrolysis of petroleum distillation residues in coil-type reactors.

Effect of feedstock on the product yields and properties of the FCC process using the feed forward NNs have been estimated by Al-Enezi and Elkamel[14]. Their designed network is capable of predicting the yields of different products including propane, n-butane, butane, iso-butane, propylene, butylene, light gas, gasoline, LCO, HCO, coke and CCR number. While API, Watson characterization factor, sulfur content, and liquid volume percent conversion are required as feed properties. They proved that their ANN model is more accurate than the commercial simulators and non-linear regression models.

A hybrid ANN model for scale up of FCC pilot plant to industrial unit has been proposed by Bollas et al[15]. The pilot model was capable to anticipate the conversion. The hybrid model was compared with the pure ANN and pilot model. The results showed that the hybrid model is more accurate than pure ANN.

Taskin et al. [16], studied Fuzzy logic control of FCC unit. FCC processes are known to be very difficult to model and control because of the complicated hydro-dynamics and complex kinetics of both cracking and coke burning reactions. They showed that fuzzy logic control, as a promising control technique, would be effectively used for improved process control of FCC in refinery process industry.

According to our literature survey, simulation and optimization study have not been performed on HOC unit using ANN and Genetic Algorithm (GA).

In this study after process description and brief introduction to ANN, the methodology for obtaining the best ANN will be described. Finally the best obtained network will be tested with unseen data. Next sensitivity analysis will be performed to find out the most affecting process parameters on gasoline production. Finally the optimization will be carried out to find optimum values of the process variables to produce maximum gasoline yield.

3.1 Catalytic cracking unit

Figure 1 shows schematic of a typical catalytic cracking process [2]. As shown in figure 1 there are three main parts in catalytic cracking processes: catalyst part, regeneration part and separation part.

Figure 1.

Catalyst part consists of a reactor or riser which chemical cracking reactions occur in the presence of catalyst in the temperature and pressure range of 500-530℃ and 2-3 bar respectively. In regeneration part catalyst surface coke is burned. The contact between reactor and regenerator cause the catalyst circulate from one container to another. Recovered heat by catalyst is saved in regenerator. Reactor outputs are transferred to separating part which includes series of distillation towers. The obtained products are full of unsaturated compounds, but they contain few unstable diolephins. [2]

According to figure 2, HOC plant includes 2 main parts, (i) catalyst part including cracking and catalyst regeneration and (ii) separation part.

Figure 2.

First vacuum gas oil (VGO), is heated in a long vertical pipe called riser and then introduced to the reactor where it is in contact to the catalyst coming from regenerator with high temperature (about 700℃). In figure 3 the schematic diagram of the HOC reactor is depicted. The feed is vaporized and is cracked due to occurring reactions and rises toward reactor riser and the pressure is kept at a low level (2 bars). The reactor temperature is stabilizes at 500℃. There is a baffle blade on the riser that carries out initial separation of hydrocarbon vapors. Catalyst drawn along with the gas is recovered in two

cyclone stages arranged in series. The products are sent to the fractionation column. The output stream which is free of catalyst is headed to the separator [1, 2, 17-20].

Figure 3.

Stripping

The bottom end part of the reactor consists of a stripper column. The vapor is injected through the catalysts to perform partial recovery of absorbed hydrocarbons. The stream passes to the stripper which is connected to the regenerator through the pipe called," standpipe". Catalyst level is controlled by a slide valve to maintain it in a fixed level [1, 2, 17-20].

Regeneration

In regeneration part, the required air flow for combustion is supplied by a blower. High-temperature combustion burns off the coke deposits from catalyst surface. Part of the combustion heat is stored by the catalyst. Regenerator catalyst off take is regulated by a slide valve. Recent catalytic cracking units are usually provided with a regenerator functioning at a high temperature (around 700℃), thereby ensuring total combustion of coke into carbon dioxide (CO_2). Such combustion is often catalyzed by adding small quantities of precious metals such as platinum to the cracking catalyst. Combustion fumes are separated from catalyst by two cyclone stage inside the regenerator. These fumes can be used to supply energy before being released into the atmosphere.

A pressure- reducing turbine can be used to recover mechanical energy, usually enough to drive the air compressor. Installation of such a turbine requires the presence of a third cyclone stage outside the regenerator, to remove catalyst "fine", thereby reducing the risk of erosion wear. After a reduction in

pressure, the fumes pass through a waste heat boiler, and the recovered sensible energy is used to generate steam.

Older units were built with regenerators operating at lower temperatures, around 620- 630 °C, since the available catalyst could not withstand heat. Regenerator fumes containe a large quantity of carbon monoxide (CO) which had to be burnt into carbon dioxide before being released into the atmosphere.Entrained catalyst is removed from the combustion gases by two stages of cyclones located in the regenerator. The high temperature flue gases are available at low pressure and can be used to produce energy before being released into the atmosphere [1, 2, 17-20].

Catalyst circulation- fluidization

The catalyst circulates at a very high rate (several tons per minute) and this is made possible by injecting oil, gas or steam into the catalyst transportation tubes. In the regenerator, catalyst fluidization is ensured by the combustion air, and by the cracked gases and the stripper steam in the reactor. Significant catalyst loss through the cyclones are observed when the particle diameter of the catalyst is in the 20-150 micron range and when 50- 70% of the catalyst grains are within the 40-80 micron bracket. [17-20].

Fractionation section

The reactor effluent is a feed of main fractionating distillation column which is in vapor form. Feed is directed to the column and the slurry recirculation which is cooled in heat exchangers. From the separator column, LCO and HCO are equipped with vapor stripper and HCO is mixed with slurry. Overhead vapors are condensed partially and some of the condensates are used in the main column.

Output gases from top of the column are compressed by compressor. This part consists of a several distillation and absorption columns for separation of the products including: fuel gas, C_3 cut (propane and propene), cut of C_4 (butane and butene), LCO, HCO [18-20].

3.2 ANN modeling

An ANN which is inspired by the biological neural system is an idea for processing the information and a highly capable tool to solve sophisticated and intricate problems like human brain. Artificial network behaves like the neural cells of human body and it is a network of complicated interconnected neurons [21]. ANNs just use the typical data set of the system, thereby the prior information of the system is unnecessary [22]. There are different ANN architectures. In this study the multilayer feed-forward neural network generally called multi layer perceptron has been designed and utilized. Figure 4 demonstrates schematic of this network. In this network I, J and K are the input, hidden and output vectors which represent the number of neurons in input, hidden and output layer, respectively [23].

Figure 4.

$$n = \left(\sum_{i=0}^{I} w_{ij}x_i\right) + b \tag{1}$$

$$\text{Hidden layer} = HL_j = f\left[\left(\sum_{i=0}^{I} w_{ij}x_j\right) + \text{bias1}\right] \tag{2}$$

$$\text{Output layer} = f\left[\left(\sum_{i=0}^{I} HL_{ij}\, w_{jk}\right) + \text{bias2}\right] \tag{3}$$

Where I is the number of elements in input vector (x_i), w_{ij} and w_{jk} are inter connected weights and b is the neuron bias. The output of each neuron is the summation of the weighted inputs and biases passing through the activation function which is calculated according to equation (3).

Generally, the ANNs are trained to receive from the spectacular input to a special target using adapting the corresponding weights. The error between the ANN outputs and targets (desired outputs) is minimized using the optimized selection of weights and biases. The training operation is stopped when the corresponding error reaches its minimum value or the number of epochs exceeds the determined epoch number. There are different ANN training algorithms. The most common training algorithm is back propagation (BP) which includes different methods and solutions. An ANN is trained using one of the BP algorithm methods and changing the weights. In this study the BP algorithm and Levenberg Marquardt (LM) method have been utilized. The supervised ANNs are trained using a set of input and output data. Weights are changed until the error between ANN output and targets meet the minimum value. The common criterion for error calculation is mean square error (MSE) which is calculated as the following: [22, 24-29]

$$MSE = \frac{1}{K}\sum_{i=1}^{K}(Z_{i,measurement} - Z_{i,simulated})^2 \quad (4)$$

Where K and Z refer to the number of outputs and their values, respectively [25-29].

4. Findings

In this research, from various designed ANN, a multi layer feed-forward using back propagation method with Levenberg Marquart (LM) algorithm was found as the best network. In order to find

optimum number of hidden neurons, the trial and error method was employed. The selection criterion was MSE between ANN outputs and test data as targets. It was found that number of hidden neurons is ten activation function of hidden layer is sigmoid function which is defined as below [24,25].

$$f(x) = \frac{1}{1 + e^{-x}} \tag{5}$$

Where x is a weighted input for neuron and $f(x)$ is an output of each neuron. The simple linear activation function is also used for the output layer as described below: [24,25]

$$f(x) = x \tag{6}$$

As mentioned before 70% of all date were used for training and 30% were employed for generalization. The percentage of relative error in generalization section is calculated based on the following equation[24,25].

$$\text{Error} = \frac{100}{K} \sum_{i=1}^{K} \left| \frac{\text{measurement} - \text{simlated}}{\text{measurement}} \right|_i \tag{7}$$

In this study eight ANNs were trained so that each network is designed for each output. The first ANN is designed for training the gasoline weight percent using all inputs and other ANNs have been constructed for weight percentage of LCO, HCO, propane, propene, iso-butane, n-butane and butane, respectively. Figure 5 (a-h) illustrate the comparison between measured and predicted outputs by

ANN for tested and trained data. For each output, network data were compared with unseen experimental data.

Figure 5.

For precise awareness, the amounts of error are shown in figures 6 (a-h). According to these figures, error percentage is between 10^{-4}-10^{-5} for different outputs, which show the high accuracy of the trained model in prediction of HOC outputs.

Figure 6.

Table 2 compares MSE (for train and test data) and regression of various algorithms. Among the BP trained networks LM algorithm had good performance and was employed for HOC process optimization.

Table 2.

4.1. Sensitivity analysis

Sensitivity analysis is an important tool to solve several problems present in many areas of human knowledge: engineering, mathematics, physics, economy, medicine, biology, etc., especially when nonlinearities are involved. Therefore, it is possible to infer about the behavior of the system face to parametric variations without the need of solving a problem that involves

complexity, described by a set of nonlinear differential and algebraic equations. The conclusions are extracted from the calculation of the derivative function under analysis [30].

A sensitivity analysis method for discovering characteristic features of the input data using NN classification models was devised. The sensitivity is the gradient of the NN model response function, and because neural network models are nonlinear, the gradient depends on the point where it is evaluated[31].

Sensitivity analysis was used to determine how the model would respond to changes in input parameters. Sensitivity analysis is acknowledged as essential for good modeling practice, and is an implicit part of any modeling field[32]. The sensitivity is quantified by the following equation:

$$\frac{\delta y}{\delta p} = \kappa \tag{8}$$

Where p, the parameter vector, is mapped into the state vector y ($p \rightarrow y$). In the present work the trained NN model is utilized as a process simulator. Because the output of a trained NN is a function of inputs alone (weights are constant after training), sensitivity analysis of a system can be conducted using the trained NN to characterize the relationship between inputs and outputs. The sensitivity of the outputs to the inputs is defined by Eq. (8), can be estimated from the trained NN model by observing the changes in the value of the k^{th} output brought about by a small change in the value of the jth input at any operating point[33].

At each operating point P, the jth input can be varied over its entire range, and the corresponding variation in the k^{th} output can be plotted to produce a sensitivity curve[33,34].

For sensitivity analysis and for evaluating the effect of changes in all inputs on each output, one of the inputs was changed in its industrial ranges while other inputs were fixed at their average values of industrial limits. The sensitivity curves of the HOC unit are illustrated in figure 7.

GA minimizes the objective function by changing the variable values randomly not according to its derivatives. Because of its stochastic identification, sticking in the local minimum is a small probable which is a good advantage of this technique but sometimes the process speed may become slow due to not handling the some of its parameters properly.[35] ANN can be used as the GA guiding function.

Heavy oil demand has decreased due to energy conservation and nuclear power development, and the demand for light products has increased. This raises the problem of the conversion of heavy products into light products such as gasoline, kerosene and diesel fuel for the production of motor fuels[17].

Regarding high consumption of gasoline as a fuel and its considerable significance and application in industry, in this study the optimization of HOC process has been performed focusing on increase in maximizing gasoline production rate.

For optimization purpose, MATLAB 7.6 GA toolbox was employed. An optimum value of the HOC gasoline function should to be searched by GA combined with the trained NN model. So, the input variables and their ranges should be determined. In the present work the volume percent of gasoline was used as an objective function to be maximized:

Objective function (J)= max(Volume percent of gasoline) (9)

In the optimization procedure, first, an initial population of 100 was used to generate 100 individuals randomly. Next, the related ANN model was called to calculate the fitness value for all generated individuals. As GA technique finds the minimum value of the fitness function, the negative of our objective function is utilized to find the maximum value for gasoline production. At the next step, three operations (selection, crossover and mutation) produce the new generation[34]. This procedure continues until the optimum value for gasoline is reached. For accurate optimization, the initial population was varied. For each initial population the optimum value of gasoline was recorded.

The obtained results are depicted in figure 8. The optimum value of the initial population is 900. More initial population may result in the accurate amount of the objective function but the computational time will be too long. To find optimum volume percent of gasoline, with 900 initial populations, 57 generation was carried out. In this case maximum volume percent of gasoline was obtained as 73.6429 LV%.

The similar calculation was performed using fmincon solver of MATLAB 7.6 optimization toolbox. The similar, 73.6459 LV%, result was obtained using fmincon solver. The optimization results are summarized in Table 3.

Table 3.

According to figure 7, sensitivity results are in a good agreement with GA. Sulfur and gas do not have any significant effect on the gasoline and as GA results show the optimum values for sulfur and gas are the lower bound of their industrial limits.

5. Conclusion

In this research an ANN model with BP method and LM training algorithm is used to simulate industrial HOC unit.. the proposed ANN was able to predict unseed industrial date accurately. The results infer high capability of ANN modelling for simulation of oil processes. Based on sensitivity analysis it was found that gasoline and HCO are more sensitive to conversion than other products, Gasoline and C_4= are more sensitive to feed API, Gasoline and HCO are more sensitive to CCR and gasoline is more sensitive to coke and HCO is more sensitive to sulfur content than other products. The optimum gasoline was found as 73.6429 and 73.6459 LV% using GA and fmincon solver, respectively.

Nomenclature

HOC	Heavy oil cracking
ANN	Artificial neural network
API	American Petroleum Institute Index
CCR	Carbon condradson residue
N-C_4	Normal butane
I-C_4	Iso-Butane
C_4=	Butene
C_3	Propane
C_3=	Propene
HCO	Heavy cycle oil
LCO	Light cycle oil
GASO	Gasoline
LM	Levenberg-Marquardt
GA	Genetic Algorithm
FCC	Fluid catalytic cracking
VGO	Vacuum gas oil
LPG	Liquid petroleum gas
I	Number of inputs in ANN
J	Number of neuron in hidden layer

K	Number of outputs in ANN
n	Total number of output, number of data
w_{ij}	Weight on the hidden layer
x	Input variable of activation function
b	Bias
f	Neuron activation function
w_{jk}	Weight on the output layer
BP	Back propagation
MSE	Mean square error
Z	Output of neuron, output layer
y	State vector
p	Parameter vector
κ	Sensitivity
Mea	Measurement data
Sim	Simulated data

6. RESEARCH OUTPUT

1. Citation Details of Articles:

- Leila Sheikhattar,Haslenda Hashim, Gholamreza Zahedi, Saeedeh Amraee, Mahdieh Abolhasani," Maximizing gasoline yield in heavy oil cracking unit", submited to Oil & Gas Science and Technology, 2010.

2. Citation Details of Conference Papers

- Hashim, H., L. Sheikhattar, G. Zahedi, " Simulation of heavy oil cracking unit", International Conference on Process Engineering and Advanced Material (ICPEAM2010)/ 24th Symposium of Malaysian Chemical Engineers (SOMChE2010), Kuala Lumpur Convention Centre, Kuala Lumpur, Malaysia, 15th-17th June 2010.
- Zahedi, G., F. Parvizian, M. R. Rahimi, "An expert model for estimation of distillation seive tray efficiency base on artificial neural network approach", International Conference on Process Engineering and Advanced Material (ICPEAM2010)/ 24th Symposium of Malaysian Chemical Engineers (SOMChE2010), Kuala Lumpur Convention Centre, Kuala Lumpur, Malaysia, 15th-17th June 2010.
- Zahedi G. , S. Saba, Ali Elkamel, H. Hashim," Prediction of ozone concentration around an industrial area using fuzzy neural network method", World Academy of Science, Engineering and Technology, 67, Bali, Indonesia, 14-16 July, 2010.

3. HUMAN CAPITAL DEVELOPMENT

- Graduate Research Assistant (GRA): RM1000 per month x 2= RM24000
- Conference: RM6000

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Appendix: tables and figures

Table 1. Variables of Neural network models.

Model variables	Limit of data
Conversion (%LV)	47.1-80.2
Feed API	16.1-29
Feed sulfur percent (%wt)	0.6-2.7
Feed CCR percent (%wt)	0.3-9.4
Feed Coke percent (%wt)	3.7-15.7
Feed Gas percent (%wt)	2.7-3.3
Product GASO percent (%LV)	27.6-62.3
Product LCO percent (%LV)	14.8-22.7
Product HCO percent (%LV)	4-30.2
Product C_3 percent (%LV)	0.6-1.9
Product C_3= percent (%LV)	1.9-9.7
Product I-C_4 percent (%LV)	0.3-5
Product N-C_4 percent (%LV)	0.4-8
Product C_4= percent (%LV)	4.1-12.1

Table 2. Comparison of MSE and Regression of various training algorithms.

Training algorithms	MSE (train)	MSE (test)	R(Regression)
traincgb	0.1993	0.1818	0.46941
traingd	3.2382	2.0212	0.77217
traingda	0.1278	0.9714	0.234
traingdm	0.1270	0.9726	0.68048
trainlm	0.0342	0.1299	1
trainoss	0.1237	0.1819	0.17816
trainrp	0.4257	0.2545	0.99575
traincsg	0.0338	0.1587	0.99768

Table 3. Optimum value of gasoline using GA and fmincon solver.

	Optimum value of gasoline (LV%)	Conversion (%)	API	Sulfur	CCR	Coke	Gas
GA*	73.6429	80.19921	25.78462	0.600165	1.572448	15.69982	2.700425
fmincon solver	73.6459	80.2	25.78564	0.6	1.572335	15.7	2.7

* Initial population=900, Generations=57

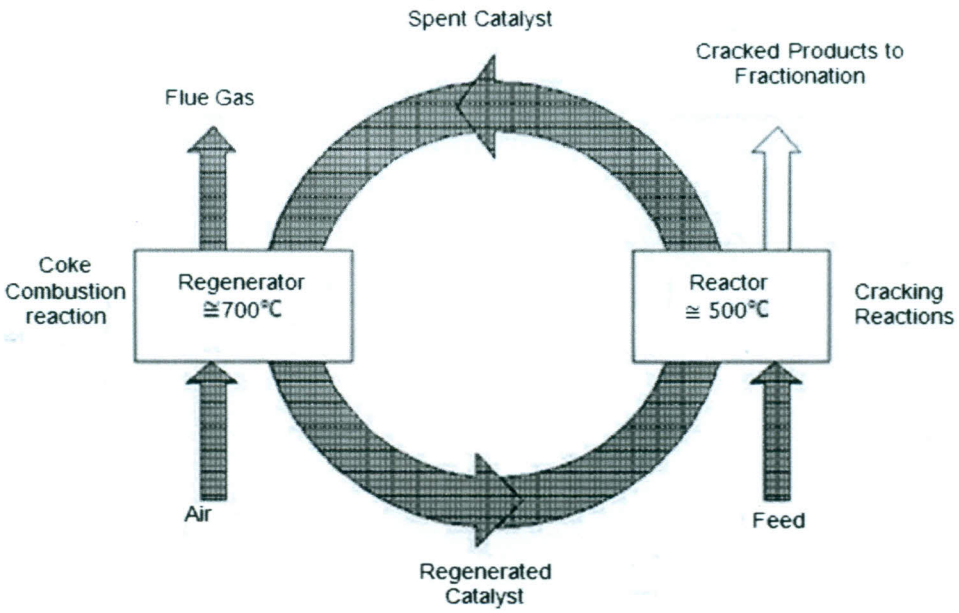


Figure 1. Schematic view of catalytic cracking processes.[17]

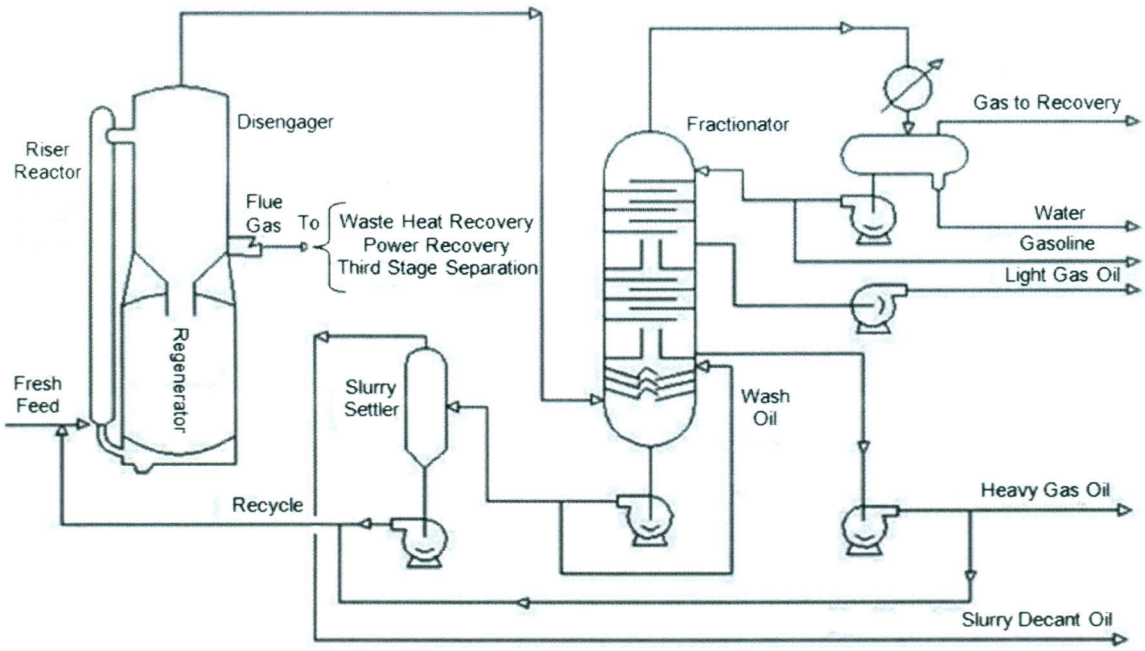


Figure 2. Schematic of HOC unit.[2]

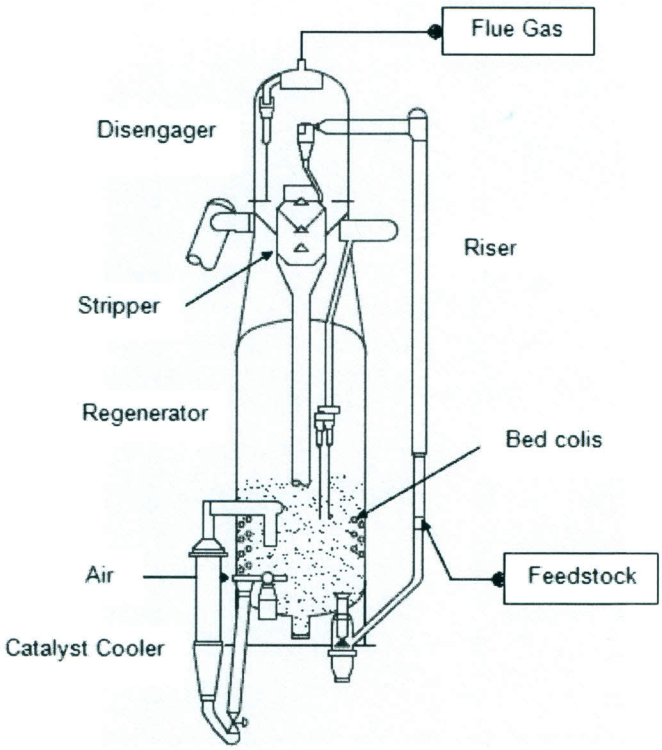


Figure 3. Schematic diagram of reactor for the HOC plant.[17]

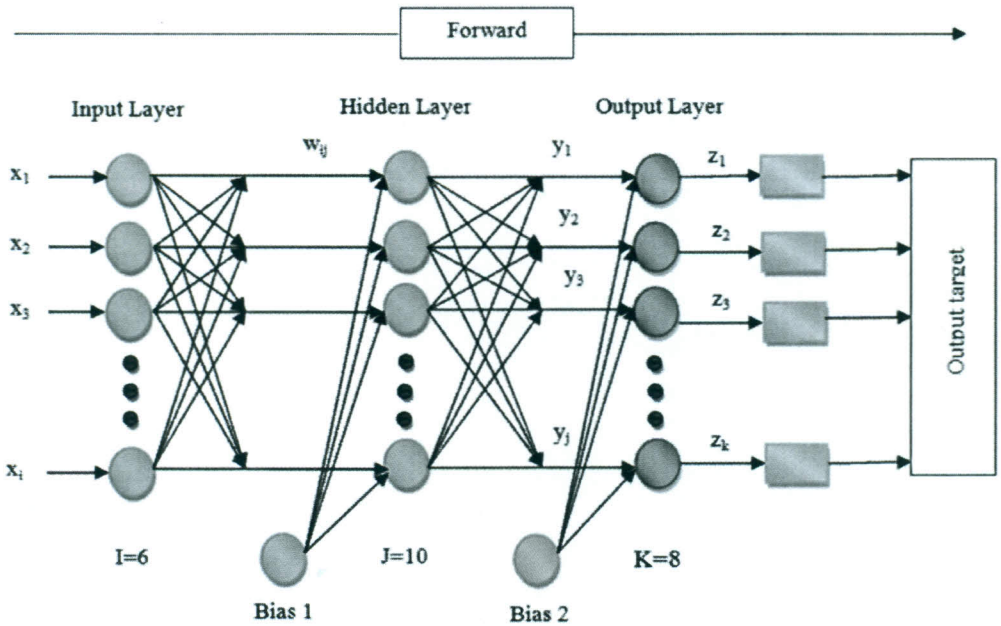


Figure 4. Schematic structure of back propagation neural network.

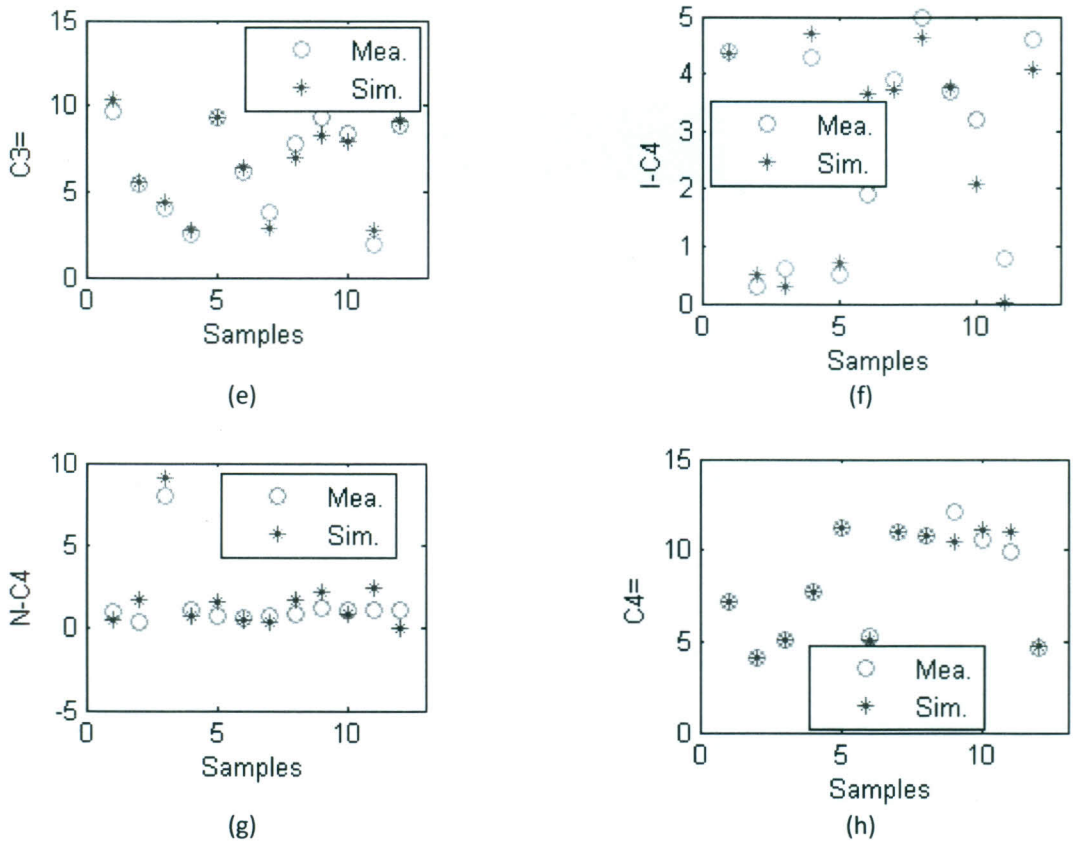
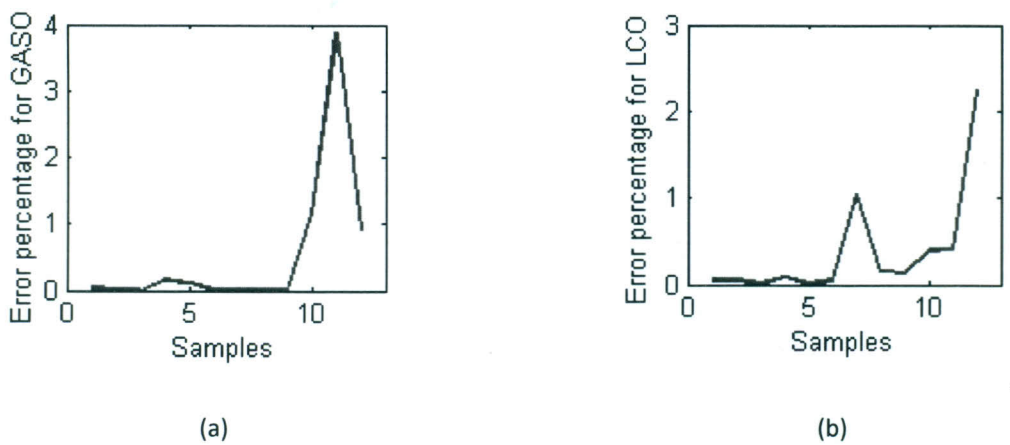


Figure 5. Comparisons between simulation results and industrial HOC output data for different products. (a) gasoline, (b) LCO, (c) HCO, (d) C_3, (e) C_3=, (f) I-C_4, (g) N-C_4, (h) C_4=



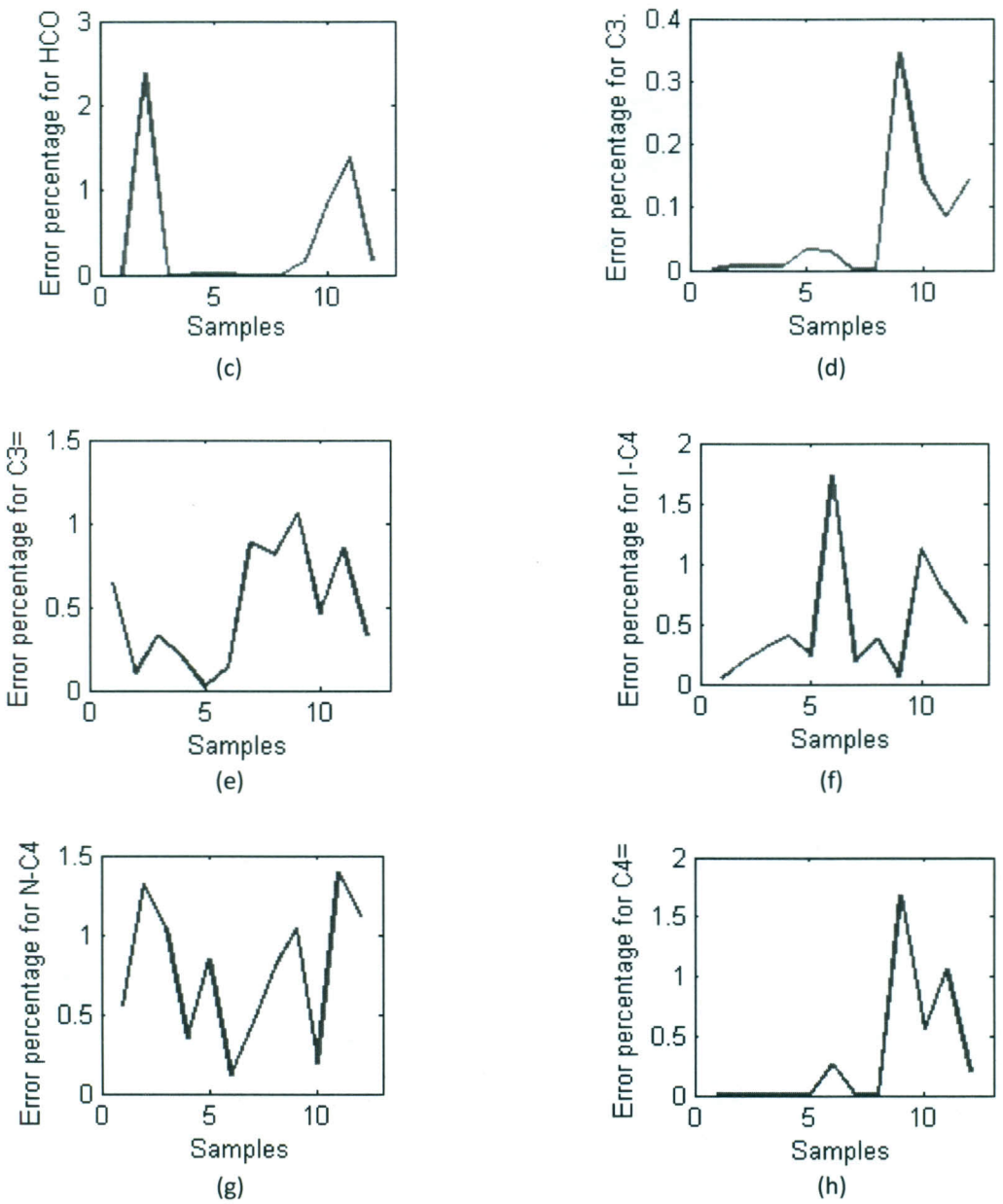


Figure 6. Error percentage between simulation results and industrial HOC output data for different products. (a) gasoline, (b) LCO, (c) HCO, (d) C_3, (e) C_3=, (f) I-C_4, (g) N-C_4, (h) C_4=

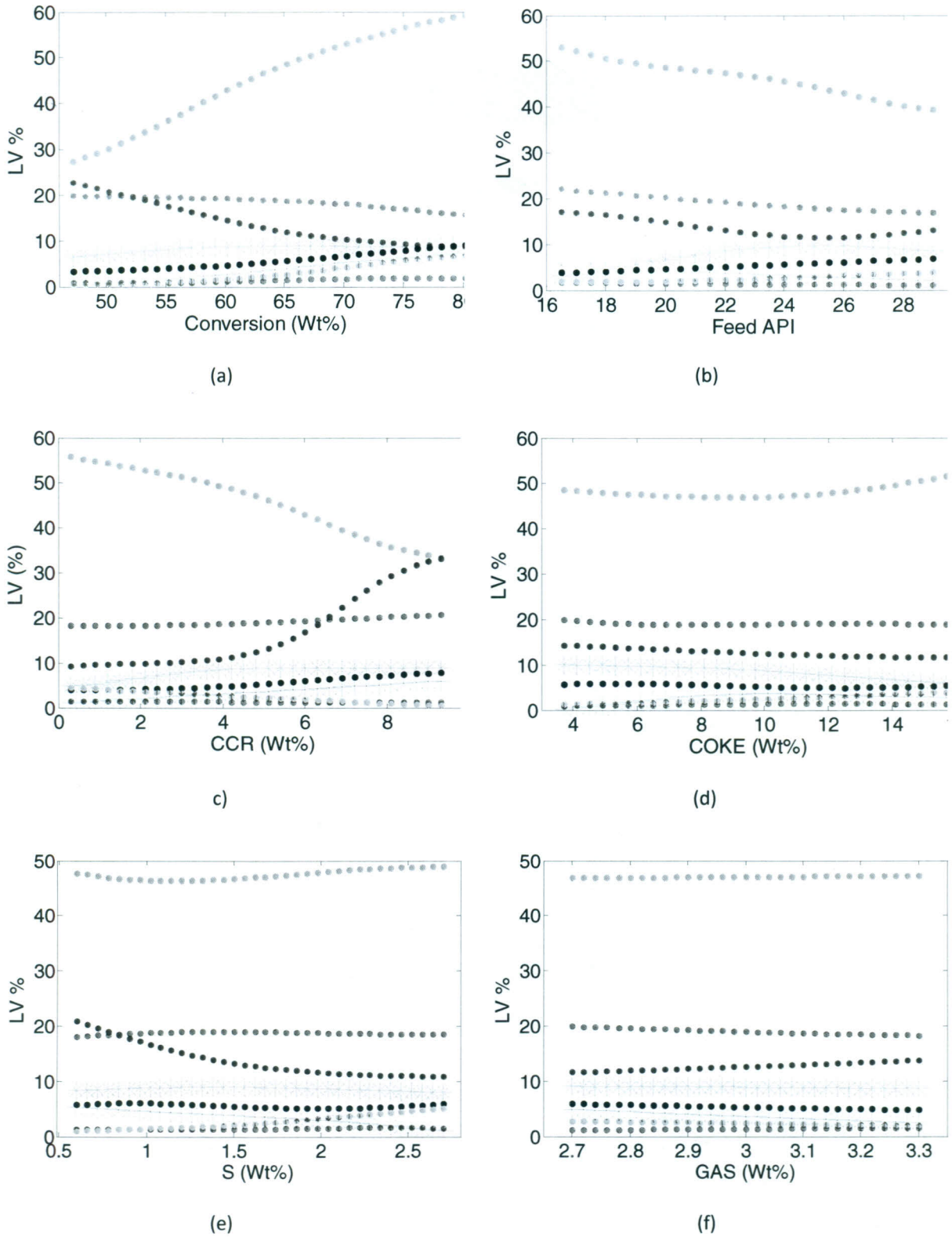


Figure 7. Sensitivity curves of HOC unit for changes in (a) Conversion percent, (b) Feed API, (c) input CCR percent, (d) input coke percent, (e) input sulfur percent and (f) input gas percent.

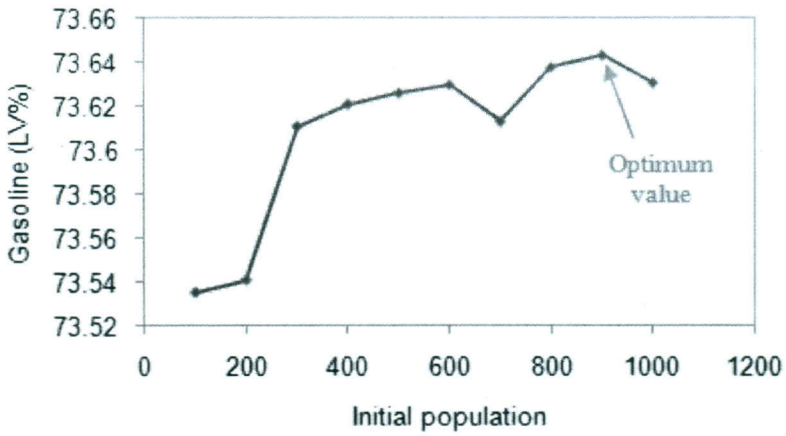


Figure 8. The trends of the volume percent of gasoline as an objective function vs. initial population.